Glutaric acid, cyclohexylmethyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C19H25ClO5/c1-23-17-12-15(20)10-11-16(17)25-19(22)9-5-8-18(21)24-13-14-

InchiKey: DOENECIGCZOQKR-UHFFFAOYSA-N

Formula: C19H25ClO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 368.85

Physical Properties

Property code	Value	Unit	Source
gf	-358.07	kJ/mol	Joback Method
hf	-805.14	kJ/mol	Joback Method
hfus	41.02	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.548		Crippen Method
mcvol	276.940	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2776.00		NIST Webbook
rinpol	2776.00		NIST Webbook
tb	902.74	K	Joback Method
tc	1127.19	K	Joback Method
tf	559.20	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.50	J/mol×K	902.74	Joback Method
cpg	881.96	J/mol×K	940.15	Joback Method
cpg	894.85	J/mol×K	977.56	Joback Method
cpg	906.18	J/mol×K	1014.96	Joback Method
cpg	915.94	J/mol×K	1052.37	Joback Method
cpg	924.16	J/mol×K	1089.78	Joback Method
cpg	930.84	J/mol×K	1127.19	Joback Method
dvisc	0.0003735	Pa×s	559.20	Joback Method

dvisc	0.0002201	Pa×s	616.46	Joback Method
dvisc	0.0001419	Pa×s	673.71	Joback Method
dvisc	0.0000980	Pa×s	730.97	Joback Method
dvisc	0.0000714	Pa×s	788.23	Joback Method
dvisc	0.0000543	Pa×s	845.48	Joback Method
dvisc	0.0000428	Pa×s	902.74	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393911&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume